

Mediated gates between spin qubits

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(Dated: July 26, 2012)

In a typical quantum circuit, non-local quantum gates are often applied to non-proximal qubits. If the underlying physical interactions are short-range (*e.g.*, exchange interactions between spins), intermediate SWAP operations must be introduced, thus reducing the efficiency of the circuit. Here we develop a new class of “mediated” gates for spin qubits, which act on non-proximal spins via intermediate ancilla qubits. At the end of the operation, the ancilla return to their initial states. We provide examples of mediated gates for a triple-quantum-dot system, and we show that these gates provide equal or improved efficiency compared to SWAP-based protocols. Our method can be extended to a spin bus, further improving the circuit efficiency.

Quantum dot spin qubits are promising candidates for quantum computing because of their long decoherence times and their potential scalability and integrability with semiconductor technologies [1, 2]. The exchange coupling is a desirable tool for mediating interactions between spin qubits, because it can be controlled electrostatically and it is typically very fast [3]. In combination with arbitrary single qubit operations, the exchange coupling enables universal quantum computation [4]. When logical qubits consist of two [5] or three [6] physical qubits in a decoherence free subsystem, the exchange coupling alone is universal for quantum computation. On the other hand, the intrinsic short-range nature of the exchange coupling (typically tens of nanometers) imposes strong constraints on the physical architecture of the spin qubits. These constraints present a significant challenge for quantum error correction [7] and scalability.

Simultaneous, many-body couplings provide a potential route for enhancing the effective range of the interactions, in analogy with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [8]. When these couplings are arranged into non-trivial topologies, such as rings, a rich spectrum of quantum gates emerges [9, 10]. However simple topologies, such as those considered here, can also lead to new types of entangling operations, which are different than the standard two-qubit gates for spin qubits.

In this paper, we show how to control such simultaneous, multi-qubit couplings. The result is a new class of “mediated” quantum gates. We focus primarily on the three-qubit geometry shown in Fig. 1, due to recent experimental progress on triple-quantum-dots [11–13]. In this arrangement, the mediated gate acts on the non-proximal qubits 1 and 2, leaving the ancilla or central qubit c unaffected, at the end of the operation. We characterize this well defined gate operation, \mathbb{U}_2 , and we show how arbitrary two-qubit states and gates can be generated using \mathbb{U}_2 as the sole entangling resource. We also compare the efficiency of these mediated-gate protocols to more conventional SWAP-based protocols. Finally, we explain how long-range mediated gates can be attained

by replacing qubit c with a spin bus.

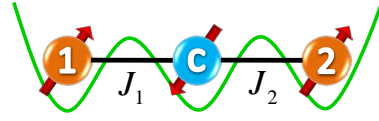


FIG. 1. (color online). A linear triple-quantum-dot geometry with three electrons. Mediated gates can be achieved between qubits 1 and 2 by applying simultaneous exchange couplings, with $J_1 = J_2$. At the end of the operation, the ancilla qubit c is restored to its initial state.

Mediated gate, \mathbb{U}_2 .—We begin by characterizing the mediated gate \mathbb{U}_2 . The effective spin Hamiltonian for the quantum dot geometry of Fig. 1 derives from the exchange interaction, and takes the form of nearest-neighbor Heisenberg couplings [4], given by

$$H = J_1 \mathbf{s}_1 \cdot \mathbf{s}_c + J_2 \mathbf{s}_2 \cdot \mathbf{s}_c, \quad (1)$$

where s_j are spin operators. In typical experiments, the coupling constants J_1 and J_2 are controlled by detuning the local electrostatic potentials in a given dot [3]. J_1 and J_2 can usually be varied independently as a function of time [11, 12]. For mediated gates, however, we assume that both couplings are turned on and off simultaneously.

The Hamiltonian H induces three-spin dynamics according to the time evolution operator $U(t) = e^{-iHt}$, where we set $\hbar = 1$. However, the mediated gate we seek has the special form $U = \mathbb{U}_2 \otimes I$, where \mathbb{U}_2 acts on qubits 1 and 2, and the identity operator I acts on the ancilla qubit c . In [14], we prove that only one non-trivial mediated gate exists for the geometry of Fig. 1, corresponding to the unique parameter combination $J_1 = J_2 = J$ and the special evolution period $T_g = 4\pi/3J$ (with periodic recurrences [15]). The gate is robust against control errors in similar fashion to conventional two-qubit exchange gates. For example, if $J_2 = J_1(1 + \delta)$ results in the gate $U(\delta)$, where $U(0)$ is the desired gate, and if the fidelity is defined as [16] $F = |\text{Tr}[U(\delta)^\dagger U(0)]|/\text{Tr}[U(0)^\dagger U(0)]$, then we obtain a quadratic error in the fidelity: $1 - F \simeq 0.97\delta^2$

when $\delta \leq 0.4$. Other mediated gates, such as the three-qubit gate \mathbb{U}_3 , can be obtained by similar methods [14].

Any unitary two-qubit operator $U_2 \in \text{SU}(4)$, including \mathbb{U}_2 , can be expressed in the form of a Cartan decomposition, given by [17, 18]

$$U_2 \stackrel{\text{l.u.}}{=} e^{\frac{i}{2}(c_1\sigma_x \otimes \sigma_x + c_2\sigma_y \otimes \sigma_y + c_3\sigma_z \otimes \sigma_z)}, \quad (2)$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices, and $\mathbf{s} = \boldsymbol{\sigma}/2$ in spinor notation. Here, the relation $\stackrel{\text{l.u.}}{=}$ means “equal, up to local unitary gates,” where the latter may be applied before or after the non-local operator. The decomposition is unique when the parameters (c_1, c_2, c_3) are restricted to the tetrahedron $\pi - c_2 \geq c_1 \geq c_2 \geq c_3 \geq 0$, known as the Weyl chamber. (Note that special considerations apply to the base of the tetrahedron [17].) There is a one-to-one mapping between the Weyl chamber and the Makhlin invariants [19], which provides an alternative representation of the non-local properties of $U_2 \in \text{SU}(4)$ (except on the bottom surface of the chamber). The Cartan decomposition for our two-qubit mediated gate is given by $(c_1, c_2, c_3) = (2, 1, 1)(\pi/3)$ and it has the explicit form [14]

$$\mathbb{U}_2 = - \begin{pmatrix} \frac{1}{2}(1+i\sqrt{3}) & 0 & 0 & 0 \\ 0 & \frac{1}{4}(-1+i\sqrt{3}) & \frac{1}{4}(3+i\sqrt{3}) & 0 \\ 0 & \frac{1}{4}(3+i\sqrt{3}) & \frac{1}{4}(-1+i\sqrt{3}) & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1+i\sqrt{3}) \end{pmatrix}. \quad (3)$$

The position of \mathbb{U}_2 in the Weyl chamber is shown in Fig. 2, along with several other common two-qubit gates.

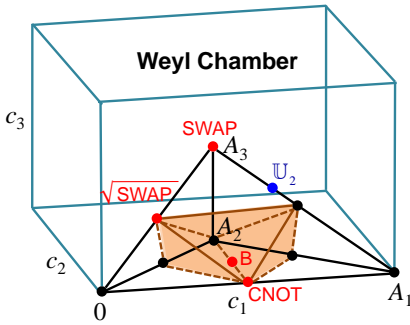


FIG. 2. (color online). A geometric representation of two-qubit $\text{SU}(4)$ gate operations, with axes c_1, c_2 , and c_3 defined in Eq. (2). The Weyl chamber corresponds to the tetrahedron $0-A_1-A_2-A_3$, while the gates known as perfect entanglers lie inside the shaded region [17]. The coordinates for other special gates are given by $B = (\frac{\pi}{2}, \frac{\pi}{4}, 0)$, $\text{CNOT} = (\frac{\pi}{2}, 0, 0)$, $\text{SWAP} = (\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2})$, and $\sqrt{\text{SWAP}} = (\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4})$.

The gating capabilities of \mathbb{U}_2 derive from its entangling properties, which are characterized in part by its position in the Weyl chamber. The operators known as “perfect entanglers” lie inside a polyhedron, which fills half of the chamber [17], as shown in Fig. 2. Combined with local unitaries, a perfect entangler can generate a maximally

entangled state from a separable state. That is, for some initial two-qubit state with concurrence [20, 21] $C = 0$, one application of a perfect entangler can produce a state with $C = 1$. The standard CNOT gate is known to be a perfect entangler [17], as indicated in Fig. 2. However, CNOT does not arise naturally from the exchange interaction between spin qubits; it must be constructed from more basic gates [4]. As we have shown, the mediated gate \mathbb{U}_2 does arise naturally in many-body spin systems; however, it is not a perfect entangler. Using the methods of [18], we find that \mathbb{U}_2 achieves a maximum concurrence of $C_{\text{max}} = \frac{\sqrt{3}}{2} < 1$ when acting upon a separable state.

A universal quantum processor must be able to generate arbitrary entangled states or implement arbitrary quantum circuits. For example, CNOT gates combined with single-qubit unitaries are known to be universal [22–24]. Any two-qubit entangling gate U_2 can replace CNOT in this scheme [25], although the entangling capabilities of the gate will affect the overall circuit efficiency. In the remainder of this paper, we explore methods for generating arbitrary entangled states and entangling gates using the mediated gate \mathbb{U}_2 , and we determine the efficiency of such protocols.

Generation of arbitrary states.—Our goal here is to construct arbitrary, two-qubit, entangled pure states between qubits 1 and 2 in the geometry of Fig. 1, using the mediated gate \mathbb{U}_2 as our non-local entangling resource. Allowing for local operations and classical communication (LOCC), it is possible to transform maximally entangled states, such as Bell states, into arbitrary pure states [26]. We therefore focus on using \mathbb{U}_2 to generate Bell states.

The strategy we adopt is to apply \mathbb{U}_2 repeatedly, assisted by single-qubit unitary rotations U_1 , as needed:

$$|\psi\rangle \stackrel{\text{l.u.}}{=} [\mathbb{U}_2(U_1 \otimes U_1)]^n |00\rangle. \quad (4)$$

Here, n represents the efficiency of the protocol. Note that each U_1 in Eq. (4) represents an arbitrary rotation, and that in general, the rotations can all be different. For other protocols, such as those involving intermediate SWAP gates, the circuit efficiency can also be expressed through n , the number of exchange gate applications. In this way, n provides a means of comparing the efficiency of disparate protocols. Since \mathbb{U}_2 is not a perfect entangler, we know that n must be greater than 1 to generate a Bell state.

We have solved Eq. (4) numerically, using global optimization methods, as described in [14]. In this procedure, the two-qubit operation \mathbb{U}_2 is fixed, and we search for the individual single-qubit rotations U_1 . In principle, the efficiency n could also vary. However, we find that maximally entangled Bell states can already be obtained when $n = 2$. The resulting circuit for the singlet Bell state $|\Psi^-\rangle$ is shown in Fig. 3(a).

We can compare our mediated-gate protocol to the

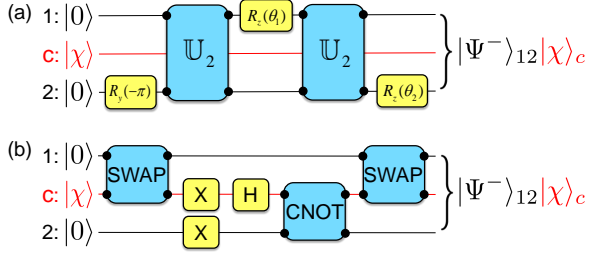


FIG. 3. (color online). (a) A quantum circuit for generating the singlet Bell state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ (up to a global phase), using the mediated gate U_2 . The single qubit rotations are represented by $R_\alpha(\theta) = e^{-\frac{i}{2}\theta\sigma_\alpha}$, where $\alpha = x, y, z$. The rotation angles here are given by $\theta_1 = -\arccos(\frac{1}{3})$, $\theta_2 = -\frac{1}{6}\pi - \arctan \frac{4\sqrt{2}-3\sqrt{3}}{5}$. Note that the ancilla state $|c\rangle$ is arbitrary, and returns to its initial state at the end of the operation. (b) An efficient Bell state protocol between non-proximal qubits, based on nearest-neighbor, pairwise gates. Here, H is the Hadamard gate and X is the Pauli gate σ_x , corresponding to a π rotation about the x -axis of the Bloch sphere (up to a global phase).

conventional Bell state protocol based on nearest-neighbor gates, as shown in Fig. 3(b). In the latter case, CNOT is used to generate the Bell state, while the SWAP gates are used to make the qubits proximal. The minimal number of exchange gates needed to construct CNOT is two [4]. Comparing Figs. 3(a) and 3(b), we obtain an exchange gate efficiency of $n = 2$ for the mediated-gate protocol and $n = 4$ for the SWAP-based protocol. The mediated gate therefore offers certain advantages for generating arbitrary states.

The Bell state protocol of Fig. 3(a) can be implemented in a triple dot system using standard experimental tools for quantum dot qubits. We now suggest a protocol for doing this, including the initialization and final verification steps. (1) Load two electrons into the singlet ground state of a single dot and separate them adiabatically into neighboring dots 1 and c using the detuning procedure described in [3]. Here, we assume that a small static, global uniform magnetic field is applied throughout the procedure, while detuning results in a configuration with $J \ll g\mu_B B$. Thus, we obtain the state $|0\rangle_1|0\rangle_c|\chi\rangle_2$, where $|0\rangle_1|0\rangle_c$ represents the ground state spin configuration, while $|\chi\rangle_2$ is an arbitrary spin state. (2) Perform a SWAP operation between dots c and 2 to obtain $|0\rangle_1|\chi\rangle_c|0\rangle_2$. This provides the initial state for the protocol of Fig. 3(a). (3) Apply the mediated-gate protocol shown in Fig. 3(a) to obtain $|\Psi^-\rangle_{12}|\chi\rangle_c$. The circuit gives the same result, with or without a uniform B -field, up to an overall phase that depends on B/J . (4) Perform a SWAP gate between dots c and 2 to obtain $|\Psi^-\rangle_{1c}|\chi\rangle_2$. (5) Perform a projective singlet measurement between dots 1 and c , as described in [3]. Note that the mediated gates U_2 , which are characterized by simultaneous couplings J_1 and J_2 , appear only in step (3) of this protocol. The other steps (1, 2,

4, and 5) are for initialization and readout purposes, and use only conventional pairwise gates.

Our goal in this section has been to efficiently generate entangled states, using the two-qubit entangling gate U_2 . To conclude the section, we note that higher-order gates such as the three-qubit mediated gate U_3 [14] can potentially provide even greater efficiency, because they are highly parallel. The global optimization techniques used to solve Eq. (4) can also be applied to this problem, by interspersing arbitrary single-qubit unitaries between the mediated gates. To demonstrate a simple but important outcome of this procedure, we have obtained a circuit that generates the maximally entangled three-qubit state GHZ_3 [27], using U_3 as the entangling resource. (See [14] for details.) Remarkably, the result can be obtained with just a single application of the mediated gate: $|\text{GHZ}_3\rangle \stackrel{\text{l.u.}}{=} U_3(U_1 \otimes U_1 \otimes U_1)|000\rangle$. In this case, the exchange gate efficiency is perfect ($n = 1$), indicating that U_3 is a perfect entangler for the three-qubit GHZ state family [27]. We can compare this to the conventional, pairwise gating circuit for GHZ_3 , which uses two CNOT gates [28]. In a quantum dot quantum computer, this would require at least four exchange gate operations, or $n = 4$.

Construction of arbitrary gates.—We now consider protocols for generating arbitrary two-qubit gates, using the mediated gate U_2 as an entangling resource, in combination with arbitrary single-qubit gates U_1 . We adopt a strategy analogous to Eq. (4), given by

$$U_2 \stackrel{\text{l.u.}}{=} [U_2(U_1 \otimes U_1)]^n. \quad (5)$$

As before, we solve this equation using global optimization techniques. The results for some familiar gates are shown in Figs. 4(a) and (c). These results (and others, described in [14]) appear to be optimal, based on exhaustive searches. None of the gates requires more than five applications of U_2 .

The mediated gate circuit for CNOT in Fig. 4(a) employs four U_2 gates. The corresponding circuit for conventional, pair-wise operations employs two $\sqrt{\text{SWAP}}$ gates when the qubits are proximal. When the qubits are non-proximal, additional SWAP gates are needed, as indicated in Fig. 4(b). Thus, for second-nearest neighbor geometry of Fig. 1, the mediated and conventional CNOT circuits have equal efficiencies ($n = 4$). We find that mediated gates are more likely to improve the efficiency of larger-size gates (*e.g.*, Toffoli), when multi-qubit entangling gates like U_3 are available, or when the central spin can be replaced with a spin bus, as discussed below.

There are several well-known techniques for constructing arbitrary two-qubit gates, which can be adapted for mediated gates. The most efficient method requires no more than two applications of the so-called B gate [29], to implement a gate whose Cartan decomposition is known. Fig. 4(c) shows our globally optimized circuit for a B gate,

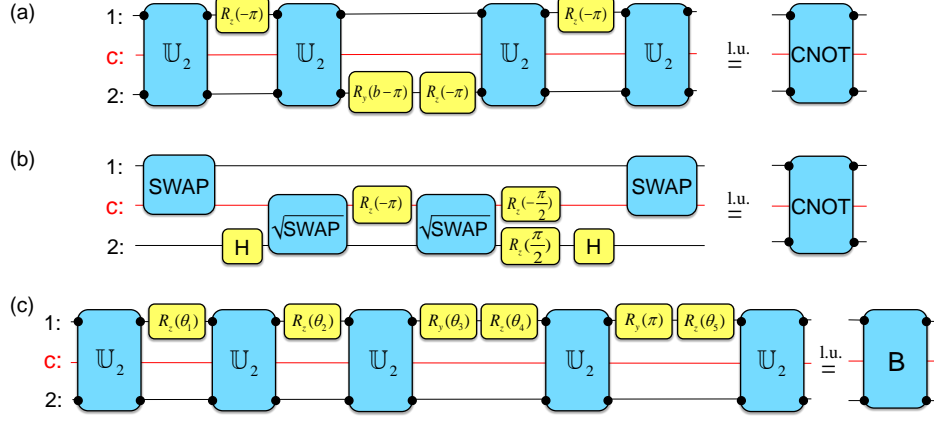


FIG. 4. (color online). (a) CNOT gate construction, based on the mediated gate U_2 . Here, $b = -\arccos(-1/3)$. (b) CNOT gate construction between non-neighboring qubits, based on nearest-neighbor pairwise gates [4]. (c) B gate construction, based on mediated gates. The circuit parameters can be obtained up to arbitrary accuracy: $\theta_1 = 0.297\pi$, $\theta_2 = 0.788\pi$, $\theta_3 = 0.660\pi$, $\theta_4 = -1.092\pi$, and $\theta_5 = 0.579\pi$. Our numerical methods give overall operator error norms of order 10^{-15} .

which employs five U_2 gates. This result (together with [29]), constitutes a formal proof that $n \leq 10$ for optimal efficiency in Eq. (5). It also forms a constructive protocol for generating an arbitrary two-qubit gate using ten U_2 gates. However, we note that the bound $n \leq 10$ does not appear to be tight, since none of the gates we have solved requires more than five applications of U_2 .

To conclude this section, we consider the scaling properties of the two-qubit mediated gate scheme for a spin bus geometry [15]. Specifically, we consider an odd-size spin chain of length N , with two external qubits. When the bus is constrained to its ground-state energy manifold, it can be treated as a spin-1/2 pseudo-spin [15]. The effective interaction between the qubits and the bus pseudo-spin has a Heisenberg form [30, 31], with an effective coupling constant $J^* \propto J/\sqrt{N}$ [15]. We can immediately extend all our three-qubit protocols, simply by replacing the central qubit in Fig. 1 with a bus, and replacing J with J^* when we calculate the gate period T_g . The resulting bus gate U_2 is identical to the two-qubit mediated gate, and the protocols proceed as before, except that the qubits can now be far apart. The exchange gate efficiency for the bus protocol is the same as for mediated gates. Specifically, it is independent of N . The gate period T_g scales as \sqrt{N} however, since $T_g \propto 1/J^*$. In contrast, the efficiency of a conventional gate protocol, based on pairwise SWAP gates, is proportional to N , while T_g is independent of N for a given pairwise operation. Thus, the spin bus architecture has much better scaling properties than the conventional gate protocol, in terms of both total gate time ($O(\sqrt{N})$ vs. $O(N)$) and circuit depth ($O(1)$ vs. $O(N)$), with immediate consequences for quantum error correction [7].

Summary.—We have developed the concept of a *mediated gate* between non-proximal qubits. The gate is implemented by coupling the qubits simultaneously through

a central, ancilla qubit, which is restored to its initial state at the end of the operation. We focus here on two-qubit gates, although three-qubit gates are also discussed (with examples given in [14]). We investigate protocols, based on global optimization techniques, for generating arbitrary states and gates, using mediated gates as the sole entangling resource. We show that a maximally entangled Bell state can be achieved with just two applications of a mediated gate, and we propose an experimental protocol for testing the procedure in a triple-quantum-dot. We also show that several important two-qubit quantum gates can be obtained using five or fewer mediated gates. We prove that ten mediated gates represent an upper bound for generating an arbitrary two-qubit gate. Finally, we note that the central ancilla qubit can be replaced by a spin bus, leading to significant improvements in scaling properties, in both total gate time and circuit depth.

We thank Jun Zhang and Andrei Galiutdinov for helpful discussions. This work was supported by the DARPA QuEST program through a grant from AFOSR, by NSA/LPS through grants from ARO (W911NF-09-1-0393 and W911NF-08-1-0482), and by NSF-PIF (PHY-1104672).

Supplemental Materials

Here, we provide details on two topics discussed in the main text. (1) We outline an existence proof for the mediated gate U_2 , when two qubits are simultaneously coupled through a central ancilla qubit. (2) We summarize details of the numerical global optimization techniques used to solve Eqs. (4) and (5) in the main text, and we mention some additional results.

I. Mediated Gates

A. Existence Proof for \mathbb{U}_2

For convenience, we now adopt slightly different notation than the main text, as indicated in Fig. 5. Here, spins 1 and 3 are the two non-proximal qubits, while spin 2 is the central ancilla qubit.



FIG. 5. Two-qubit mediated gate geometry. Here, the ancilla qubit 2 mediates the gate \mathbb{U}_2 , which acts on qubits 1 and 3.

We consider the following Hamiltonian for a linear three-qubit array:

$$H = J_a \mathbf{s}_1 \cdot \mathbf{s}_2 + J_b \mathbf{s}_2 \cdot \mathbf{s}_3, \quad (\text{S1})$$

where \mathbf{s}_j is the spin operator for qubit j . In principle, J_a and J_b may take any value. However, we limit our search to the case where the couplings are turned on and off simultaneously. J_a and J_b are therefore constant throughout the gate operation. The goal of this subsection is to identify specific relations between J_a and J_b that lead to mediated gates.

We will make use of the identity [32]

$$4\mathbf{s}_i \cdot \mathbf{s}_j = 2p^{ij} - I, \quad (\text{S2})$$

where p^{ij} is the SWAP (i.e., permutation) operator between spins i and j , and I is the two-qubit identity operator. Hamiltonian (S1) can then be rewritten as

$$H = \frac{1}{2}(J_a p^{12} + J_b p^{23}) - \frac{1}{4}(J_a + J_b). \quad (\text{S3})$$

The time evolution operator is given by

$$\begin{aligned} U(t) &= e^{-iHt} \\ &= e^{i(J_a+J_b)t/4} e^{-iQJ_b t/2} \\ &= e^{i(J_a+J_b)t/4} \sum_{n=0}^{\infty} \frac{(-iJ_b t/2)^n}{n!} Q^n, \end{aligned} \quad (\text{S4})$$

where $\hbar = 1$ and we have defined

$$Q \equiv p^{23} + Jp^{12}, \quad (\text{S5})$$

with $J = J_a/J_b$. Since p^{23} and p^{12} are generators of the symmetric group S_3 , we may expand Q^n in terms of the S_3 group elements:

$$Q^n = a_n p^{231} + b_n p^{312} + c_n p^{12} + d_n p^{13} + e_n p^{23} + f_n I. \quad (\text{S6})$$

Here, p^{ijk} is the tripartite, cyclic permutation operator.

TABLE I. Cayley table for the symmetric group S_3 .

	I	p^{12}	p^{13}	p^{23}	p^{231}	p^{312}
I	I	p^{12}	p^{13}	p^{23}	p^{231}	p^{312}
p^{12}	p^{12}	I	p^{231}	p^{312}	p^{13}	p^{23}
p^{13}	p^{13}	p^{312}	I	p^{231}	p^{23}	p^{12}
p^{23}	p^{23}	p^{231}	p^{312}	I	p^{12}	p^{13}
p^{231}	p^{231}	p^{23}	p^{12}	p^{13}	p^{312}	I
p^{312}	p^{312}	p^{13}	p^{23}	p^{12}	I	p^{231}

The full set of S_3 group operations is given in Table. I. We then deduce the recursion relations for $Q^{n+1} = QQ^n$:

$$a_{n+1} = c_n + Jd_n, \quad (\text{S7})$$

$$b_{n+1} = d_n + Je_n, \quad (\text{S8})$$

$$c_{n+1} = a_n + Jf_n, \quad (\text{S9})$$

$$d_{n+1} = b_n + Ja_n, \quad (\text{S10})$$

$$e_{n+1} = f_n + Jb_n, \quad (\text{S11})$$

$$f_{n+1} = e_n + Jc_n. \quad (\text{S12})$$

Forming the coefficients into a column vector,

$$\mathbf{v}_n = [f_n \ c_n \ e_n \ a_n \ b_n \ d_n]^T, \quad (\text{S13})$$

the recursion relations can be expressed as

$$\mathbf{v}_{n+1} = T\mathbf{v}_n, \quad (\text{S14})$$

where

$$T = \begin{pmatrix} 0 & J & 1 & 0 & 0 & 0 \\ J & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & J & 0 \\ 0 & 1 & 0 & 0 & 0 & J \\ 0 & 0 & J & 0 & 0 & 1 \\ 0 & 0 & 0 & J & 1 & 0 \end{pmatrix}. \quad (\text{S15})$$

We now solve the recursion problem analytically. The $n = 0$ term of the summation in Eq. (S4) corresponds to the initial condition $\mathbf{v}_0 = [1 \ 0 \ 0 \ 0 \ 0 \ 0]^T$. Equation (S14) then leads to

$$a_n = \frac{1}{3}[(1+J)^n - (1-J+J^2)^{\frac{n}{2}}], \quad (\text{S16})$$

$$b_n = \frac{1}{3}[(1+J)^n - (1-J+J^2)^{\frac{n}{2}}], \quad (\text{S17})$$

$$f_n = \frac{1}{3}[(1+J)^n + 2(1-J+J^2)^{\frac{n}{2}}], \quad (\text{S18})$$

$$c_n = d_n = e_n = 0, \quad (\text{S19})$$

when n is even, and

$$c_n = \frac{1}{3}[(1+J)^n + (2J-1)(1-J+J^2)^{\frac{n-1}{2}}], \quad (\text{S20})$$

$$d_n = \frac{1}{3}[(1+J)^n - (1+J)(1-J+J^2)^{\frac{n-1}{2}}], \quad (\text{S21})$$

$$e_n = \frac{1}{3}[(1+J)^n + (2-J)(1-J+J^2)^{\frac{n-1}{2}}], \quad (\text{S22})$$

$$a_n = b_n = f_n = 0, \quad (\text{S23})$$

when n is odd. Performing the sum over n , the time

evolution operator can finally be written as

$$\begin{aligned}
 U(t) = \frac{e^{iJ_b t(1+J)/4}}{3} & \left\{ p^{231} \left[\cos(J_b t(1+J)/2) - \cos(J_b t \sqrt{1-J+J^2}/2) \right] + p^{312} \left[\cos(J_b t(1+J)/2) - \cos(J_b t \sqrt{1-J+J^2}/2) \right] \right. \\
 & + I \left[\cos(J_b t(1+J)/2) + 2 \cos(J_b t \sqrt{1-J+J^2}/2) \right] - ip^{12} \left[\sin(J_b t(1+J)/2) + \frac{2J-1}{\sqrt{1-J+J^2}} \sin(J_b t \sqrt{1-J+J^2}/2) \right] \\
 & - ip^{13} \left[\sin(J_b t(1+J)/2) - \frac{1+J}{\sqrt{1-J+J^2}} \sin(J_b t \sqrt{1-J+J^2}/2) \right] \\
 & \left. - ip^{23} \left[\sin(J_b t(1+J)/2) + \frac{2-J}{\sqrt{1-J+J^2}} \sin(J_b t \sqrt{1-J+J^2}/2) \right] \right\}. \quad (S24)
 \end{aligned}$$

The mediated gates we search for can be decomposed as

$$U = \mathbb{U}_2 \otimes I, \quad (S25)$$

where \mathbb{U}_2 acts on qubits 1 and 3, while I is the single-qubit identity operator acting on spin 2. Condition (S25) is satisfied when the coefficients of p^{231} , p^{312} , p^{12} , and p^{23} in Eq. (S24) all vanish. The solution is given by

$$J = \frac{J_a}{J_b} = 1, \quad (S26)$$

with

$$\cos(J_b t/2) = \cos(J_b t), \quad (S27)$$

$$\sin(J_b t/2) = -\sin(J_b t). \quad (S28)$$

The latter two equations determine the mediated gate periods, $t = T_g$, corresponding to

$$J_b T_g = 0, \frac{4\pi}{3}, \frac{8\pi}{3}, 4\pi, \dots \quad (S29)$$

The time evolution obtained from Eq. (S26)(S27)(S28) is given by

$$U(T_g) = e^{iJ_b T_g/2} [I \cos(J_b t) - ip^{13} \sin(J_b T_g)]. \quad (S30)$$

Equation (S29) then leads to three distinct types of gate operations. When $J_b T_g = (4m)\pi$, with m an integer, we obtain the trivial gate, $U(T_g) = I$. When $J_b T_g = (4m + \frac{4}{3})\pi$, we obtain the non-trivial result

$$U(T_g) = e^{-i\frac{\pi}{3}} \left(\frac{1}{2}I - i\frac{\sqrt{3}}{2}p^{1,3} \right). \quad (S31)$$

The decomposition of Eq. (S25) leads to the identification of the mediated gate,

$$\mathbb{U}_2 = - \begin{pmatrix} \frac{1}{2}(1+i\sqrt{3}) & 0 & 0 & 0 \\ 0 & \frac{1}{4}(-1+i\sqrt{3}) & \frac{1}{4}(3+i\sqrt{3}) & 0 \\ 0 & \frac{1}{4}(3+i\sqrt{3}) & \frac{1}{4}(-1+i\sqrt{3}) & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1+i\sqrt{3}) \end{pmatrix}. \quad (S32)$$

When $J_b T_g = (4m + \frac{8}{3})\pi$, we obtain the complementary gate $U(T_g) = \mathbb{U}_2^2 \otimes I$. Finally, we note that $\mathbb{U}_2^3 = I$. Thus, \mathbb{U}_2 , \mathbb{U}_2^2 , and I comprise the full set of two-qubit mediated gates.

B. Three-Qubit Mediated Gate, \mathbb{U}_3 .

We now consider the mediated gate geometry shown in Fig. 6, with three qubits coupled via a single mediating spin, c . For this larger geometry, the group theoretical methods of Supplemental Sec. I.A are cumbersome. However, we can still identify mediated gates by making an assumption analogous to Eq. (S26), that the couplings to the three qubits are all equal. The Hamiltonian is then given by

$$H = J(\mathbf{s}_1 \cdot \mathbf{s}_c + \mathbf{s}_2 \cdot \mathbf{s}_c + \mathbf{s}_3 \cdot \mathbf{s}_c), \quad (S33)$$

and the time evolution operator is given by $U(t) = e^{-iHt}$.

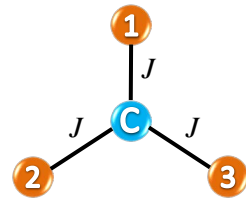


FIG. 6. Three-qubit mediated gate geometry. Here, ancilla qubit c mediates the gate \mathbb{U}_3 , which acts on qubits 1-3.

We can solve $U(t)$ numerically, and then search for gate periods $t = T_g$ for which the mediated gate decomposition, $U = \mathbb{U}_3 \otimes I$, occurs. Here \mathbb{U}_3 is the mediated gate acting on qubits 1-3, while I is the single-qubit identity acting on spin c . This procedure leads to four different mediated gates [15]. The first gate is the trivial identity operator, which occurs at the gate periods $JT_g = (8m)\pi$. The second gate occurs at the gate peri-

ods $JT_g = (8m + 2)\pi$, and takes the form

$$\mathbb{U}_3 = i \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/3 & 2/3 & 0 & 2/3 & 0 & 0 & 0 \\ 0 & 2/3 & -1/3 & 0 & 2/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/3 & 0 & 2/3 & 2/3 & 0 \\ 0 & 2/3 & 2/3 & 0 & -1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2/3 & 0 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 2/3 & 0 & 2/3 & -1/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{S34})$$

The third gate occurs at the gate periods $JT_g = (8m + 4)\pi$, and is given by $\mathbb{U}_3^2 = -I$. The fourth gate occurs at the gate periods $JT_g = (8m + 6)\pi$, and is given by $\mathbb{U}_3^3 = -\mathbb{U}_3$.

II. Constructing States and Gates with \mathbb{U}_n

A. Global Optimization

Our protocol for generating arbitrary states and gates with \mathbb{U}_2 is summarized in Eqs. (4) and (5), respectively, in the main text. To summarize, an arbitrary quantum circuit is formed of units comprised of one entangling gate, \mathbb{U}_2 , sandwiched between single-qubit unitary rotations. One or more of these units are combined, sequentially, to form a circuit. The single-qubit rotations in this protocol are arbitrary. However, the entangling gate \mathbb{U}_2 is fixed, with the form shown in Eq. (S32).

Three scalar parameters are required, to fully specify an arbitrary single-qubit rotation, up to a global phase factor (*e.g.*, the Euler angle construction). Following convention [23], we adopt the ZYZ decomposition:

$$U_1(\alpha, \beta, \gamma) = e^{-i\alpha\sigma_z/2} e^{-i\beta\sigma_y/2} e^{-i\gamma\sigma_z/2}. \quad (\text{S35})$$

In the most general case, the rotations will be applied to both qubits, at every exchange gate. Up to $6(n + 1)$ rotation angles are therefore required, to specify an arbitrary gate sequence of length n .

Here, we employ global optimization techniques, to search through this large parameter space. We have found that multi-start clustering algorithms [33, 34] are particularly effective for solving this problem. We first define an appropriate objective function to be minimized. For generating arbitrary states, as in Eq. (4), we use the infidelity $(1 - f)$ of the desired final state $|\psi_{\text{des}}\rangle$ as the objective function, where

$$f = |\langle\psi_{\text{des}}|\psi_{\text{actual}}\rangle|^2 \quad (\text{S36})$$

$$= |\langle\psi_{\text{des}}|(U_1 \otimes U_1)[\mathbb{U}_2(U_1 \otimes U_1)]^n|00\rangle|^2.$$

For generating arbitrary gates, as in Eq. (5), we use the operator error norm ϵ as the objective function, where

$$\epsilon = \|U_{2,\text{des}} - U_{2,\text{actual}}\|. \quad (\text{S37})$$

The global optimization is performed in two steps. In the first step, we use the multi-start algorithm to identify potential candidate solutions. Then, we use these solutions as a first guess in a local Nelder-Mead downhill simplex search [35]. The final outcome generally provides results with very low or very high accuracy. The latter are accepted as valid solutions. We begin our searches using the minimal exchange gate sequence ($n = 1$). If no valid solutions are obtained for a given sequence length, we increment n by 1 and repeat the procedure. Once an optimal, numerical solution has been obtained, it is sometimes possible to work backwards, to determine the exact rotation angles, as in Figs. 3, 4, and 8. These identifications are then confirmed analytically.

B. Two-Qubit SWAP Gates

In the main text, we describe global optimization results, using mediated gates to generate a Bell state (Fig. 3), a CNOT gate (Fig. 4(a)), and a B gate (Fig. 4(c)).

In Figs. 7(a) and (b), we also provide results for SWAP and $\sqrt{\text{SWAP}}$ gates, respectively.

C. Three-Qubit Circuits

The methods used to generate two-qubit states and gates can also be extended to three-qubit problems. However, three-qubit protocols are slightly more complicated because they can use two-qubit gates, three-qubit gates, or both. The most general scheme for generating a three-qubit state is shown in Fig. 8(a).

There are two non-fungible forms of entanglement for three qubits [27]. The two categories are characterized as W states, with $|W_3\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$, and GHZ states, with $|\text{GHZ}_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. The GHZ state is understood to be maximally entangled for three qubits. We have applied the global optimization protocol to obtain $|\text{GHZ}_3\rangle$ and $|W_3\rangle$, as shown in Figs. 8(b) and (c). Remarkably, we find that the GHZ state can be attained with just one application of \mathbb{U}_3 , indicating that \mathbb{U}_3 is a perfect entangler for this family of states. It is interesting to note that \mathbb{U}_3 is locally equivalent to the time evolution operator for the three-qubit triangular geometry (evaluated at a special time) [36]. The latter gate is also capable of generating $|\text{GHZ}_3\rangle$ in a single time step.

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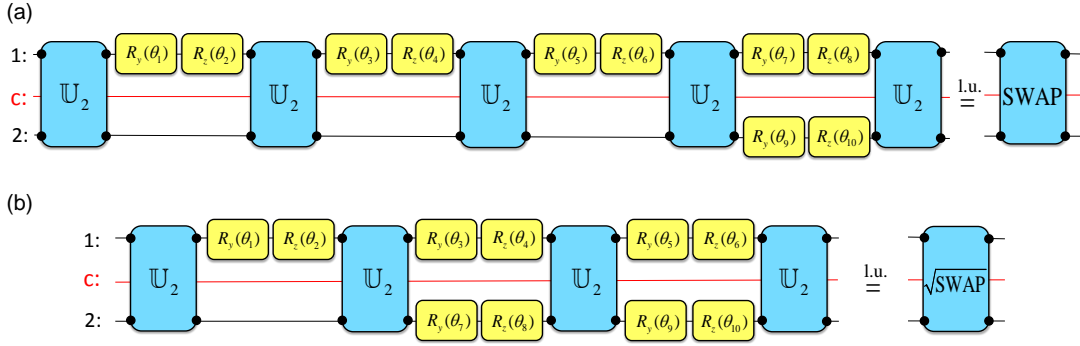


FIG. 7. (a) Global optimization results for a SWAP gate. The parameters are $\theta_1 = -0.737\pi$, $\theta_2 = -0.465\pi$, $\theta_3 = -0.543\pi$, $\theta_4 = 0.700\pi$, $\theta_5 = 0.807\pi$, $\theta_6 = 0.009\pi$, $\theta_7 = -0.278\pi$, $\theta_8 = 0.369\pi$, $\theta_9 = 0.274\pi$, and $\theta_{10} = -0.325\pi$. (b) Global optimization results for a $\sqrt{\text{SWAP}}$ gate. The parameters are $\theta_1 = 0.524\pi$, $\theta_2 = 0.549\pi$, $\theta_3 = 1.015\pi$, $\theta_4 = 0.100\pi$, $\theta_5 = 0.392\pi$, $\theta_6 = -0.305\pi$, $\theta_7 = -0.437\pi$, $\theta_8 = 0.626\pi$, $\theta_9 = -0.906\pi$, and $\theta_{10} = -0.174\pi$. For both cases, the value of the parameters can be obtained with arbitrary accuracy, and the overall operator error norm ϵ can be of order 10^{-14} .

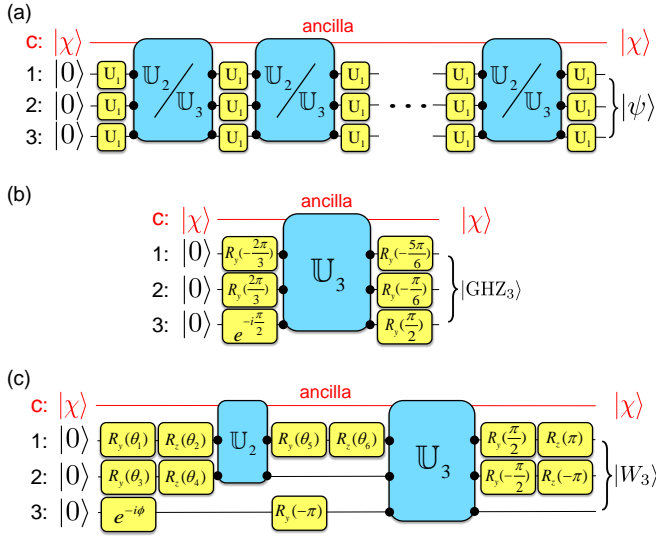


FIG. 8. (a) A general circuit for generating an arbitrary three-qubit state, using U_2 and/or U_3 gates. Note that U_2 can act on different pairs of qubits. (b) Circuit for generating a $|\text{GHZ}_3\rangle$ state, using the three-qubit mediated gate U_3 . (c) Circuit for generating a $|\text{W}_3\rangle$ state, using both U_2 and U_3 gates. The parameters in the circuits are $\theta_1 = -0.262\pi$, $\theta_2 = 0.730\pi$, $\theta_3 = -1.356\pi$, $\theta_4 = 0.349\pi$, $\theta_5 = 1.193\pi$, $\theta_6 = 0.270\pi$, and $\phi = 1.299\pi$. The value of the parameters can be obtained with arbitrary accuracy. The infidelity for this result ($1 - f$) can be of order 10^{-15} . In (a)-(c), we note that the central ancilla spin c mediates the multi-qubit gates, as shown in Fig. 6, although it returns to its initial state at the end of the operation; we therefore include c in the circuit diagram and use black dots to indicate the qubits whose interactions it mediates.

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